Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Reply to "A further study of acetylacetone nitrosation"

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Kinetic traces in the absence of added-catalyst at increasing AcAc concentrations

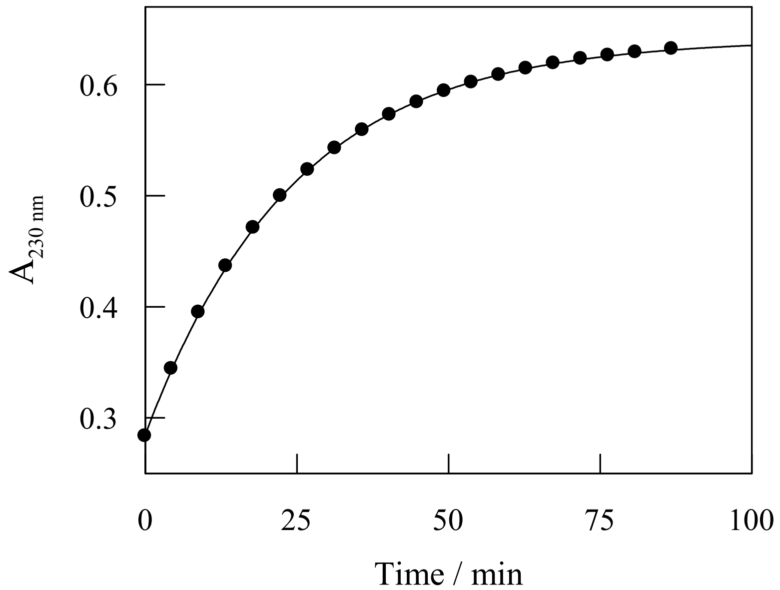

Figure S1. Fit of the absorbance-time data at 230 nm to the integrated first-order rate law, $A_t=A_\infty-(A_\infty-A_0)\exp(-k_{obs}t)$ where $k_{obs}=(6.852\pm0.031)\times10^{-4}$ $s^{-1.}$ [AcAc]=5.3×10^{-4} M; $[H^+]$=0.13 M; $[NaNO_2]$=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC. KO

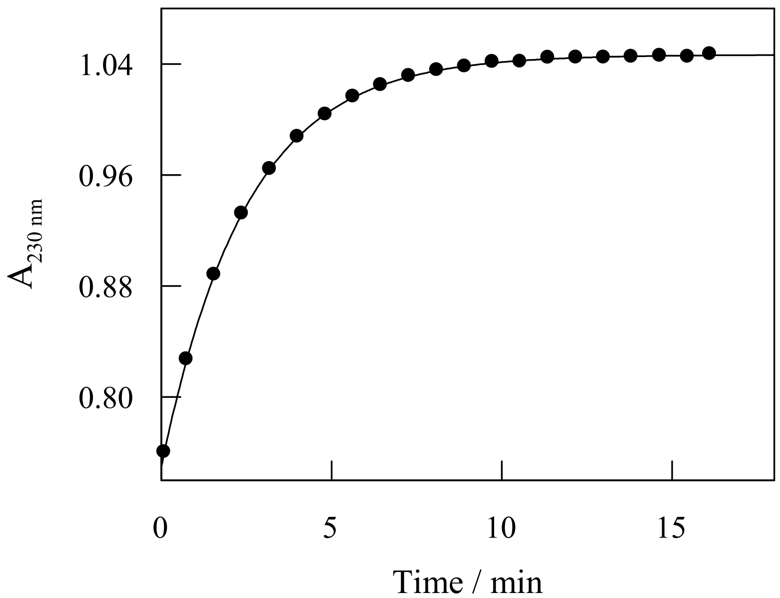

Figure S2. Fit of the absorbance-time data at 230 nm to the integrated first-order rate law, $A_t=A_\infty-(A_\infty-A_0)\exp(-k_{obs}t)$ where $k_{obs}=(6.700\pm0.024)\times10^{-3}$ s^{-1}. [AcAc]=5.3×10^{-3} M; $[H^+]$=0.13 M; $[NaNO_2]$=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.

Kinetic traces in the absence of added-catalyst at increasing acid concentrations

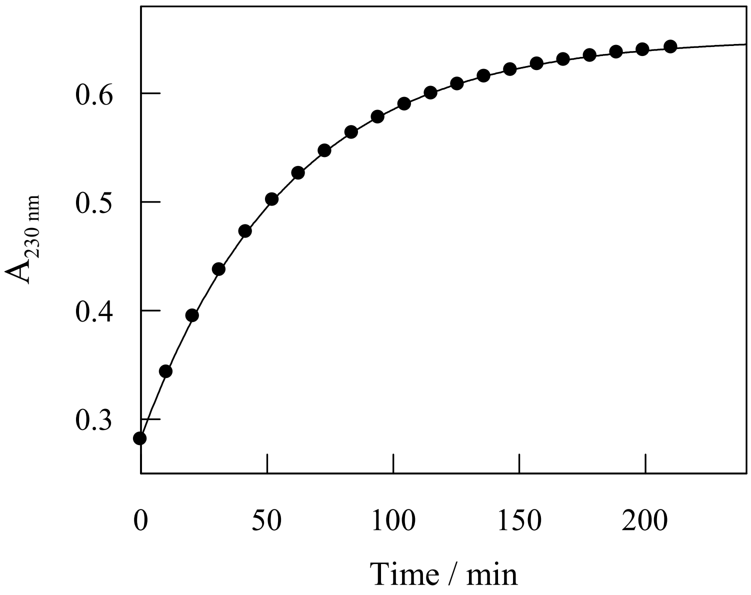

Figure S3. Fit of the absorbance-time data at 230 nm to the integrated first-order rate law, $A_t = A_\infty - (A_\infty - A_0)\exp(-k_{obs}t)$ where $k_{obs} = (2.870 \pm 0.013) \times 10^{-4}$ s^{-1}. [AcAc]=5.3×10^{-4} M; [H^+]=0.055 M; [$NaNO_2$]=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.

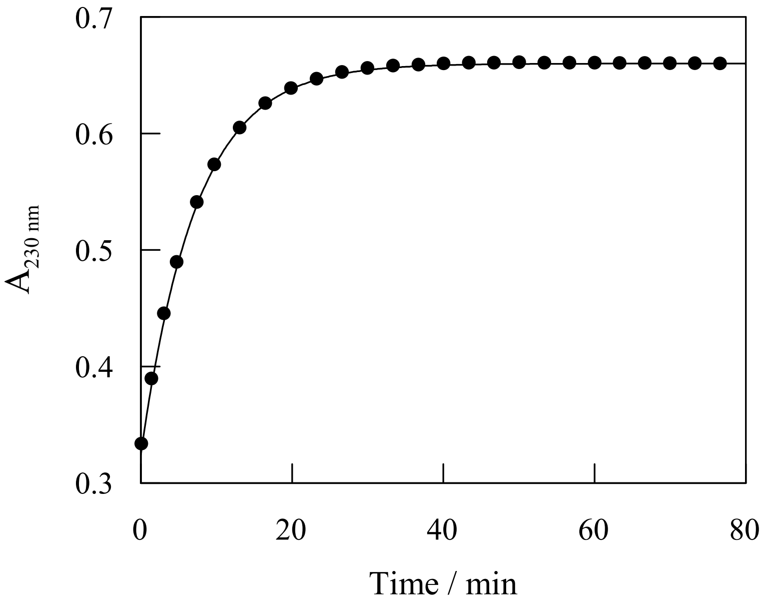

Figure S4. Fit of the absorbance-time data at 230 nm to the integrated first-order rate law, $A_t = A_\infty - (A_\infty - A_0)\exp(-k_{obs}t)$ where $k_{obs} = (2.285 \pm 0.008) \times 10^{-3}$ s^{-1}. [AcAc]=5.3×10^{-4} M; [H^+]=0.50 M; [$NaNO_2$]=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.

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Kinetic traces in the presence of nucleophiles

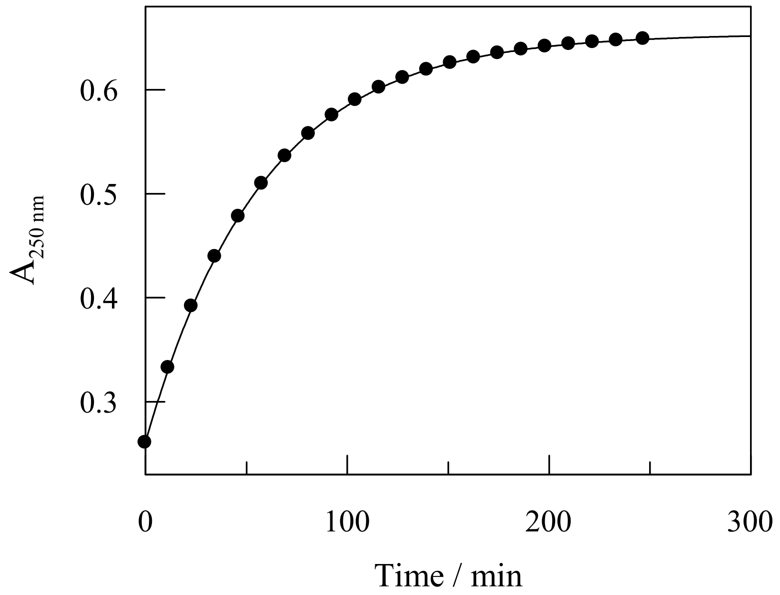

Figure S3. Fit of the absorbance-time data at 250 nm to the integrated first-order rate law, $A_t = A_\infty - (A_\infty - A_0)\exp(-k_{obs}t)$ where $k_{obs} = (2.895 \pm 0.007) \times 10^{-4}\ s^{-1}$. [AcAc]=$5.3 \times 10^{-4}$ M; [Cl^-]=0.10 M; [H^+]=0.052 M; [$NaNO_2$]=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.

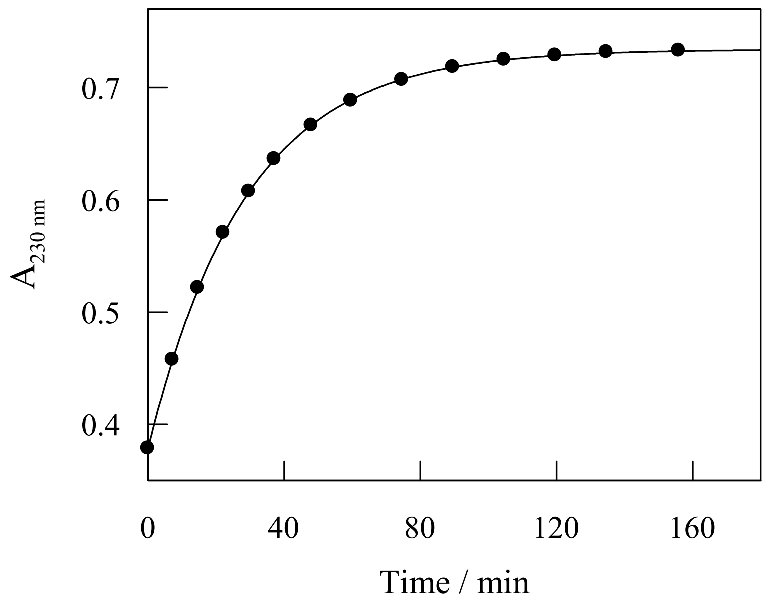

Figure S4. Fit of the absorbance-time data at 230 nm to the integrated first-order rate law, $A_t = A_\infty - (A_\infty - A_0)\exp(-k_{obs}t)$ where $k_{obs} = (5.775 \pm 0.020) \times 10^{-4}\ s^{-1}$. [AcAc]=$5.3 \times 10^{-4}$ M; [Br^-]=0.05 M; [H^+]=0.052 M; [$NaNO_2$]=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.

Kinetic traces in the presence of buffer solutions

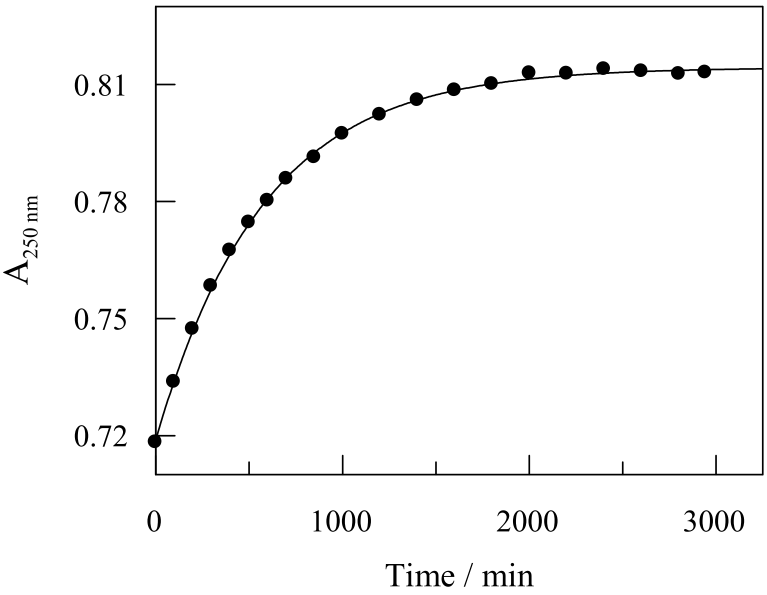

Figure S5. Fit of the absorbance-time data at 250 nm to the integrated first-order rate law, $A_t = A_\infty - (A_\infty - A_0)\exp(-k_{obs}t)$ where $k_{obs} = (2.898 \pm 0.040) \times 10^{-5}\ s^{-1}$. [AcAc]=$5.3 \times 10^{-4}$ M; [MCA]=0.10 M; pH=2.23; [$NaNO_2$]=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.

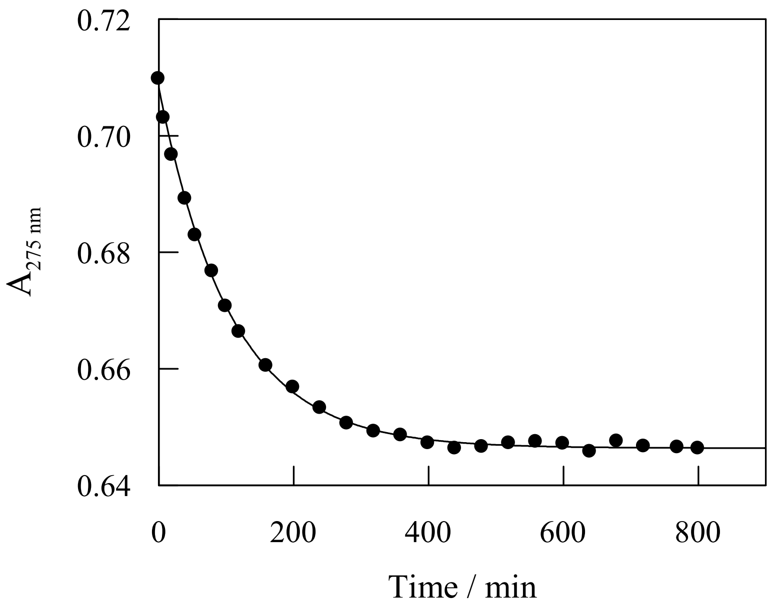

Figure S6. Fit of the absorbance-time data at 275 nm to the integrated first-order rate law, $A_t = A_\infty - (A_\infty - A_0)\exp(-k_{obs}t)$ where $k_{obs} = (1.560 \pm 0.029) \times 10^{-4}\ s^{-1}$. [AcAc]=$5.3 \times 10^{-4}$ M; [DCA]=0.50 M; pH=1.75; [$NaNO_2$]=5.0×10^{-5} M; Ionic strength 1.0 M ($NaClO_4$); T=25.0 ºC.